Doppler Broadening as a Lower Limit to the Angular Resolution of Next Generation Compton Telescopes

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ABSTRACT

The angular resolution of a telescope which detects gamma-rays via the Compton effect is fundamentally limited below a few hundred keV by the fact that the target electrons have an indeterminable momentum inside their atoms which introduces an uncertainty in the recoil energy of the Compton electron and the scattered photon. This additional component in the energy and momentum equation results in a Doppler broadening of the angular resolution compared to the standard Compton equation for a target at rest. The deterioration in resolution is most pronounced for low photon energy, high scatter angle, and high Z of the scatter material. This physical limit to the angular resolution of a Compton telescope is present even if all other parameters (e.g. energy and position) are measured with high accuracy. For different Compton scatter materials such as silicon, germanium and xenon, which are used in current telescope designs, the best possible angular resolution as a function of photon energy and scatter angle is calculated. Averaged over all scatter angles and energies, the Doppler-limited angular resolution of silicon is a factor of ~ 1.6 better than that of germanium and a factor of ~ 1.9 better than that of xenon. Looking at the Doppler limit of materials from Z=1 to 90 the best angular resolution can be reached for alkaline and alkaline earth metals, the worst for elements with filled p-orbitals (noble gases) and d-orbitals (e.g. Pd and Au). Of all semiconductors which might be used in a next generation Compton telescope, silicon seems to be the best choice.

Keywords: Gamma-Ray Astronomy, Compton Scattering, Doppler Broadening, Angular Resolution

1. INTRODUCTION

With the development of the next generation of Compton telescopes, which should cover a larger energy band and provide much better energy resolution than their predecessor COMPTEL¹, the angular resolution is slowly converging towards its lower limit, which is determined by the momentum distribution of the bound electrons in the scatter material.

Compton scattering describes the coherent interaction of photons with electrons. In 1923 Arthur Holly Compton² assumed the target electron to be free and at rest and derived his well-known Compton equation from energy and momentum conservation:

$$\cos \varphi = 1 - \frac{E_0}{E_g} + \frac{E_0}{E_g + E_e} \tag{1}$$

Here φ is the scatter angle of the photon, E_0 is the rest energy of an electron, E_e the energy of the recoil electron and E_g is the energy of the scattered gamma-ray.

A few years later Klein and Nishina derived the Compton cross section for unpolarized photons scattering off unbound electrons:

$$\left(\frac{d\sigma}{d\Omega}\right)_{ub\ C} = \frac{r_e^2}{2} \left(\frac{E_g}{E_i}\right)^2 \left(\frac{E_g}{E_i} + \frac{E_i}{E_g} - \sin^2\varphi\right) \tag{2}$$

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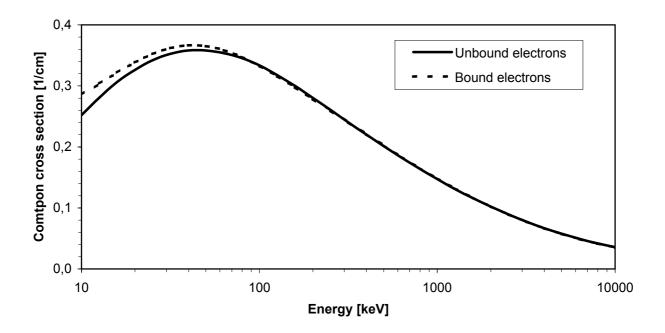


Figure 1. Compton cross section for the bound and unbound Compton scattering in silicon: While both curves are almost identical at energies above several 100 keV, for lower energies Compton scattering on bound electrons has a slightly higher probability than on unbound electrons.

Here r_e is the classical electron radius and E_i is the initial energy of the photon. Equation 2 is also called the *unbound Compton* cross section.

Unfortunately, in a real life detector system the electrons are neither free nor at rest, but bound to a nucleus. So in 1929 Jesse DuMond³ interpreted a measured broadening of Compton spectra as Doppler broadening induced by the velocity of the electrons.

Therefore a more sophisticated Compton cross section was needed to take into account the momentum distribution of the bound electrons. An expression for this effect has been derived by Roland Ribberfors⁴ in 1975:

$$\left(\frac{d\sigma}{d\Omega}\right)_{bC,i} = \left(\frac{d\sigma}{d\Omega}\right)_{ubC} S_i^I (E_i, \varphi, Z) \tag{3}$$

Here S_i^I is the incoherent scattering function of the i-th shell electrons in the impulse approximation, as it has been calculated by Ribberfors⁵ in 1982, and Z is the atomic number of the scattering material. This equation is called the *bound Compton* cross section.

Compared with Compton scattering on free electrons at rest three consequences arise:

- Obviously the total scatter probabilities change (Fig. 1): Especially at lower energies, photons have a slightly higher probability to scatter than predicted by the Klein-Nishina equation (Equ. 2) for unbound electrons.
- The scatter angle distribution changes (Fig. 2): Compared to the Klein-Nishina equation small and large scatter angles are slightly suppressed. This effect is reduced for higher energies.

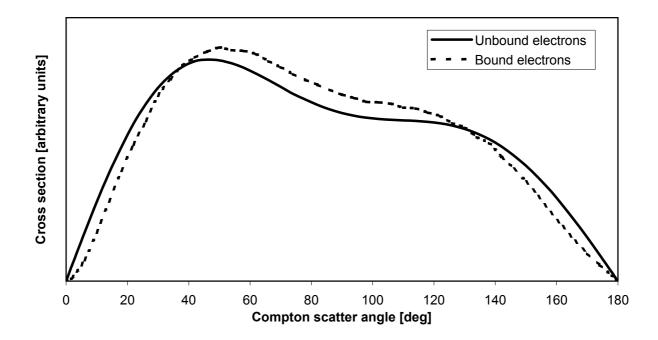


Figure 2. Compton cross sections for the bound and unbound Compton scattering as a function of the Compton scatter angle at 100 keV. Both areas are normalized to 1. In the bound case small and large scatter angles are slightly suppressed.

• The energy distribution between recoil electron and scattered gamma-ray changes. As a consequence the measured scatter angle and the one calculated with the standard Compton equation (Equ. 1) differ, which leads to broadened lines in the energy spectra for fixed scatter angles. Therefore this effect is widely known as *Doppler broadening*.

For a Compton telescope the first two points have little impact other than slightly modifying the event distributions and total sensitivity for lower energies. But since there is no way to determine the momentum of the electron, the third point gives rise to a lower limit of the angular resolution of Compton scattering-based telescopes.

Since we are only interested in the lower limit of the angular resolution we now assume ideal detectors, which have absolute accuracy in their measurement of energy and position. Moreover, all photons are completely absorbed within the sensitive detector material and all background events can be rejected. In the following analysis we will give our focus to the materials silicon, germanium and xenon, since for all of them prototypes for next generation Compton telescopes exist or are planned (e.g. Si: MEGA⁶ and TIGRE⁷, Ge: "Germanium Compton Telescope" (GCT)⁸, Xe: LXeGRIT⁹).

The following results were obtained by simulations with a modified version of the GEANT3 Low Energy Compton Scattering (GLECS v3.2) package by Marc Kippen. GLECS is based on the implementation of Doppler broadening for EGS4. For the limitations of the implementation see Namito¹⁰ (e.g. impulse approximation, all atoms are assumed to be free).

2. DOPPLER-BROADENED ANGULAR RESOLUTIONS

One possibility for characterizing the angular resolution of a Compton telescope is the so-called Angular Resolution Measure (ARM). It is the distribution of the minimum angular distance between the (known) real origin of a photon (point source) and the reconstructed origin. It can be calculated as the difference between the

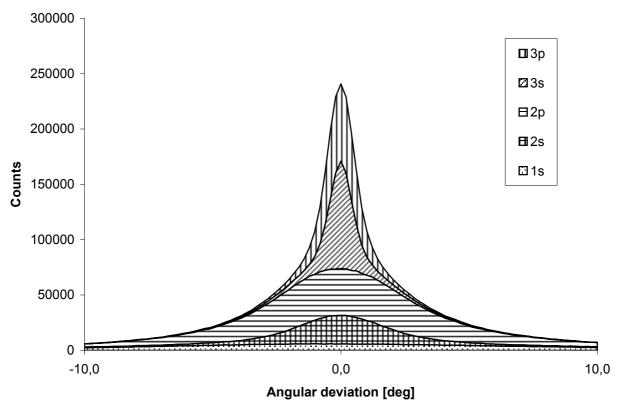


Figure 3. Cumulative ARM profile (see explanations for Equ. 4) of silicon for photons at 200 keV with no scatter angle selections. The different areas represent the contributions of different shells of the silicon atom: in the outside shells, the electrons are less energetic and closer to the "target-at-rest" assumption. Therefore the distribution is sharper. Remark: For very large scatter angles the Doppler-broadened energies of electron and scattered gamma-ray sometimes do not fit to a Compton process described by Equ. 1. These events were omitted. Except for that, the areas represent the number of electrons in the individual orbitals.

geometrical scatter angle (angle between the direction of the initial \vec{r}_i and the scattered photon \vec{r}_g) and the scatter angle calculated with the Compton equation:

$$ARM = \{ \angle (\vec{r}_i, \vec{r}_g) - \varphi \quad \forall \text{ photons} \}$$
 (4)

As the angular resolution we have chosen the FWHM of the ARM distribution, despite the wide tails of the distribution (see Fig. 3), since the peak of the distribution determines the angular resolution of a final image and the long tails only contribute to background. This angular resolution is the resolution of the telescope, not the resolution of the final image. There, effects like statistics, background, distance to the next point source, image reconstruction technique, etc. play an important role, so that the image resolution may be better or worse

An example for the shape of a Doppler-broadened ARM profile for silicon is shown in Fig. 3. The total profile is composed of the profiles of the different shells: the innermost electrons (1s orbital) have the highest momentum, and therefore the widest distribution. The 2p orbital is populated by 6 electrons, whereas all other orbitals consist of two electrons. For this reason the 2p orbital contributes most to the width of the profile. The outermost electrons have the lowest momentum and therefore form the peak of the distribution. The FWHM of the ARM-profiles has been determined by fitting a superposition of five Lorentz functions $(f(\varphi) = \sum_{i=1}^{5} \frac{a_i}{b_i^2 + \varphi^2})$ in order to resolve the shell structure, i.e. the sharp peaks as well as the wide tails of the distribution. Even for high Z materials this seems to be a good approximation.

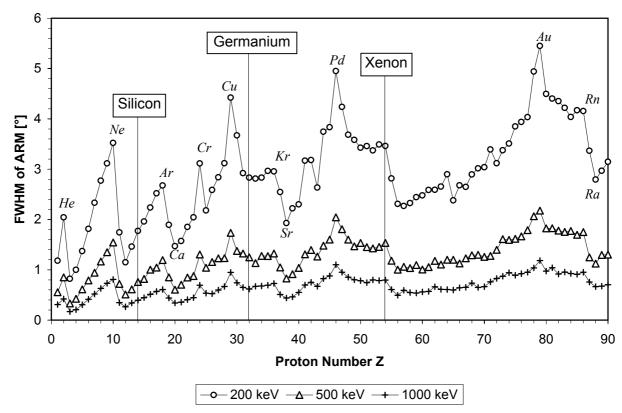


Figure 4. Dependence of the angular resolution on the nuclear charge. The best angular resolution is obtained for alkaline or alkaline earth metals. The worst FWHM is reached when orbitals are completely filled (e.g. for noble gases).

From Equ. 3 it should be obvious that the Doppler-limited angular resolution depends on three parameters: the initial photon energy E_i , the Compton scatter angle φ and the atomic number Z.

Figure 4 presents the dependence of the angular resolution on the atomic number. On average, the angular resolution worsens with increasing Z. But it also strongly depends on the shell structure of the individual atoms. Up to calcium (Z=20) the relationship is simple: it increases until it reaches a noble gas (He, Ne, Ar), then the FWHM decreases and reaches a minimum at the alkaline metals or alkaline earth metals. However, for higher atomic numbers the noble gases krypton, xenon and radon are only smaller local maxima. The three highest local maxima around Z=30, Z=46 and Z=79 are reached when the 3d, 4d and 5d orbitals are filled for the first time. For example, Pd-46 is the maximum, and not Cd-48, because of its special electron configuration: the two electrons from the 5s orbital are filling the 4d orbital. Similar reasons can be found for other extraordinary local maxima, e.g. for Cr-24 the 3d orbital is half filled.

Of the most important detector materials, silicon has the best angular resolution assuming ideal detector properties, followed by germanium and finally the noble gas xenon. Nevertheless, from the Doppler broadening

Material	Si	MgS	Ge	CdTe	Xe	NE213	CsI	NaI
FWHM at 200 keV [degree]	1.80	1.90	2.85	3.50	3.30	1.75	2.95	3.00
FWHM at 500 keV [degree]	0.80	0.80	1.25	1.55	1.45	0.75	1.25	1.40
FWHM at 1000 keV [degree]	0.40	0.45	0.65	0.85	0.80	0.40	0.75	0.85

Table 1. Doppler broadening of different semiconductor materials, xenon and scintillators.

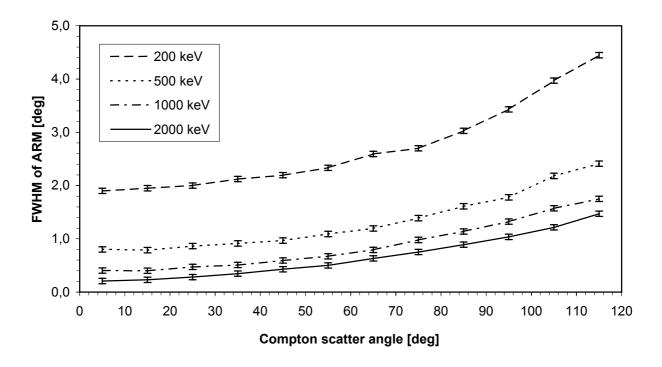


Figure 5. Dependence of the angular resolution on the Compton scatter angle φ for germanium at four energies. All values are averaged within 10°-bins.

point of view a Compton telescope based on alkaline or alkaline earth metals would be the best choice. Since a modern Compton telescope scatter material should preferably be a semiconductor in order to get a high energy and spatial resolution, one possibility could be to use II-VI semiconductors. But there are two important draw backs: Most of the II-VI semiconductors do not consist of alkaline earth metals but of transition elements with an appropriate electron configuration (e.g. CdTe), and materials like MgS suffer from their second compound: If one compares magnesium and sulfur with silicon, then the FWHM of sulfur is almost the same amount worse than silicon as magnesium is better than silicon. Therefore the net differences according to Doppler broadening between Si and MgS are marginal. Furthermore, scintillators like NaI, which consist of a low-Z and a high-Z compound, are dominated by the high-Z material because of its larger number of electrons and can therefore not benefit from their alkaline metal component. Table 1 summarizes the performance of different semiconductor and scintillator materials. Some hydrocarbon-based scintillators like NE213, which was used as the scatter material in COMPTEL, have a slightly better performance than silicon due to their hydrogen component.

The angular resolution also strongly depends on the Compton scatter angle φ (see Fig. 5). The FWHM worsens with larger scatter angles and therefore with smaller energy of the scattered photon. This behavior can be explained with Eqn. (5):

$$\Delta \varphi = \frac{E_0}{\sin \varphi} \frac{\Delta E}{E_g^2} \tag{5}$$

Here $\Delta \varphi$ is the uncertainty of the scatter angle (i.e. the width of the ARM) as a function of the uncertainty of the energy ΔE , which is the difference between the measured energy of the scattered gamma-ray with and without Doppler broadening. Equation 5 is the first derivative of the Compton equation (Equ. 1) with respect to the energy of the scattered gamma-ray E_g (E_i is assumed to be constant since Doppler broadening only changes the distribution of energy between electron and gamma-ray compared to the standard Compton equation and not the total energy). It reaches its minimum for small scatter angles and so does the angular resolution (despite the $\sim 1/\sin \varphi$ dependence).

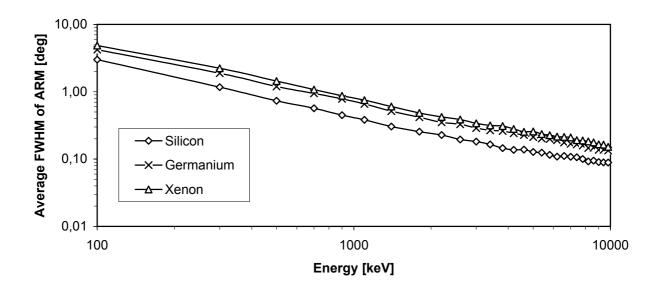


Figure 6. Dependence of the angular resolution on the energy of the initial gamma-ray. The values are averaged in 200 keV intervals below 1100 keV and in 400 keV intervals above 1100 keV. No event selections were applied.

Figure 6 summarizes the relationship between the initial photon energy and the angular resolution: On average silicon has a resolution roughly 1.6 times better than that of germanium and roughly 1.9 times than that of xenon. All three curves roughly fit a power law with $\alpha = -0.75$.

3. CONCLUSIONS

Doppler broadening is a fundamental limit for the angular resolution of Compton scattering-based telescopes below roughly 1 MeV. Unfortunately, it invalidates several strategies to improve Compton telescopes at these energies:

Due to their stopping power high Z materials (e.g. Ge, CdTe, Xe) are favored in gamma-ray astronomy. They guarantee a high efficiency, but their angular resolution is fundamentally limited. In particular germanium Compton telescopes cannot take advantage of their good energy resolution, since they have already reached their Doppler limit⁸ at lower energies.

From the Doppler broadening point of view a Compton telescope should be based on silicon since it can achieve the best angular resolution. But, on the other hand, silicon needs much more material to achieve the same efficiency and in current implementations the energy resolution is worse than in germanium telescopes. Nevertheless, if in the future it becomes possible to substantially improve the energy resolution of silicon, the resolving power for close sources of a Si-based telescope should be much better than that of a system based on germanium or other high-Z materials.

For Tracking Compton telescopes like MEGA⁶, the scatter angle dependence of the Doppler broadening seems to be a disadvantage, since an electron needs a certain amount of energy to pass through several layers of material. The required amount of electron energy corresponds to a bias towards larger scatter angles. But since a reasonable amount of tracking sets in at roughly 1-2 MeV¹¹ of the initial gamma-ray, and since those detectors are based on silicon, Doppler broadening in the current implementations is not a limiting factor.

Another drawback are the wide tails of the angular distributions. They represent additional background which has to be rejected by appropriate methods, and they make it more difficult to resolve sources in crowded fields, e.g. in the galactic center region.

At the moment no way is known to overcome the Doppler limit. Therefore below roughly 1 MeV Compton telescopes cannot give a better angular resolution than modern coded mask systems like $IBIS^{12}$ on board INTEGRAL, which has an angular resolution of roughly 0.2° . Even an ideal silicon-based Compton telescope will not reach this value below 1-2 MeV, depending on the event selections (compare Fig. 5 and 6).

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